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Mechanism of the reaction of 2-methoxybenzo[d][1,3,2]dioxaphosphinin-4-one with chloral by quantum-chemical calculations

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Abstract

Quantum-chemical calculations of various stereoisomers, intermediates, and transition states of the reaction of 2-methoxybenzo[d][1,3,2]dioxaphosphinin-4- one with chloral, leading to formation of 2-methoxy-3-(trichloromethyl) benzo[e[1,4,2λ5]dioxaphosphepin-2,5-dione, were carried out by the density functional theory (DFT) method with the PBE functional and Triple z basis, using the Priroda program. The first step of the reaction is [1+2] cycloaddition of phosphorus to the chloral C=O bond to form an intermediate with a five-coordinate phosphorus atom via a transition state in which the positive and negative charges are strongly localized on phosphorus and chloral oxygen, respectively. Calculations of the internal reaction coordinate from all transition states were carried out.

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